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A Model of Concrete Carbonation Using Comsol Multiphysics®

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Overview

- Concrete carbonation
- Physical model
- Equations
- Boundary conditions
- Results
- Conclusions

Concrete carbonation

- CO_2 permeates the porous and fractured structure of concrete.
- Establishes conditions of concrete degradation.
- Controls reinforcing bar corrosion and durability of the whole civil structure.
- May cause corrosion around reinforcing bars, causing deterioration of material and structure mechanical properties.

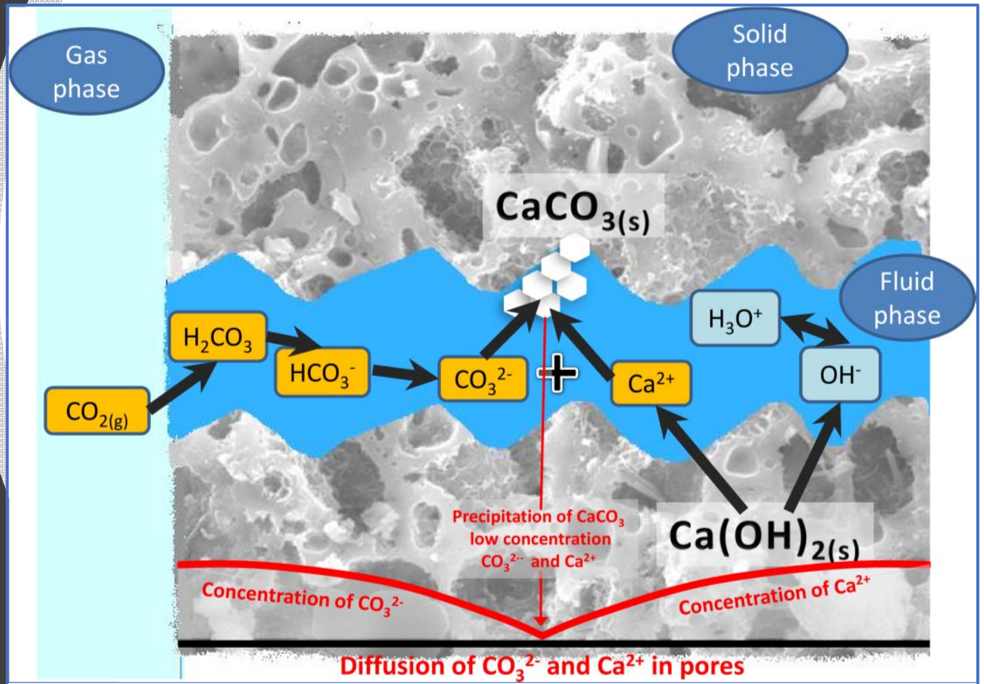


Figure 1. Carbonation of an OPC, validated also for pozzolanic cements [Papadakis et al, 1992]

Physical model

- 10 cm diameter and 20 cm height cylinders.
- Two base surfaces covered with aluminum foil to set up a radial diffusion process.
- Pozzolanic cement MP/A-28 manufactured by Lafarge-Holcim.

Table 1. Chemical composition of Lafarge-Holcim MP/A-28 cement.

Specie	Content (%)
MgO (Magnesium oxide)	2.19
SO_3 (Sulphur trioxide)	2.51
C_3A (Tricalcium aluminate)	8.30
C_3S (Tricalcium silicate)	62.40
C_2S (Dicalcium silicate)	12.50
C_4AF (Tetracalcium aluminoferrite)	9.30

Table 2. Chemical composition of the pozzolanic addition.

Specie	Content (%)
SiO_2 (Silicon dioxide)	83.6
Al_2O_3 (Aluminum oxide)	0.2
Fe_2O_3 (Iron dioxide)	1.6
CaO (Calcium oxide)	0.8
MgO (Magnesium oxide)	0.1
SO_3 (Sulphur trioxide)	0.9
K_2O (Potassium oxide)	0.0
Na_2O (Sodium oxide)	0.2

- Water to binder w/c and aggregate to binder a/c ratios were 0.52 and 4.17, respectively.
- Samples were cured for 90 days in a wet chamber at 23±2 ^{o}C and at relative humidity higher than 95%.

- Samples placed in accelerated carbonation chamber.
- Water is the solvent for the chemical reactions.
- CO_2 diffusion mechanism is set in the radial direction.
- Velocity of carbonation front depends on CO_2 effective diffusivity.
- Diffusion coefficient is a function of water/cement (w/c) ratio and degree of saturation of pores with water [Papadakis *et al*, 1989; Papadakis *et al*, 1992].
- XRD confirms calcium aluminosilicate presence in the pozzolanic cement and of anorthite $CaAl_2Si_2O_8$ in sands used to prepare the concrete blend. No $Ca(OH)_2$ was detected.

Mathematical model

- Comsol Multiphysics® Chemical Reaction Engineering Module.
- Transient, bi-dimensional diffusion mechanism for species transport.
- Convective processes are neglected, isothermal conditions are assumed.
- Chemical species are considered to be diluted.
- Porosity and water saturation in concrete are considered constant.
- Results are validated by comparing with experimental testing.
- We assume a carbonation reaction in the liquid phase between calcium aluminosilicates and CO_2 gas:

$$CO_2 + CaAl_2Si_2O_8 + 2H_2O = CaCO_3 + AlSi_2O_5(OH)_4 \quad (1)$$

[Oelkers *et al*, 2008]

Equations

- The partial differential equation for the mass conservation of a chemical specie i in a time dependent, diffusion transport process in a liquid of a partially filled saturated porous media is:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D\nabla c_i) = R_i \qquad (2)$$

For the reacting specie i of Eq. 2, c_i is its concentration, D is the diffusion coefficient and R_i is the reaction rate expression.

- The above equation is obtained by writing the conservation of the mass flux vector N_i of the specie i, starting with Fick's 1st law for diffusion of species in a diluted solution, and in absence of convective mechanisms:

$$-D\nabla c_i = N_i \qquad (3)$$

Table 3. Molar masses, densities and diffusion coefficient of the reacting chemical species of Eq. 1.

Specie	Molar mass (g/mol)	Density (kg/m^3)	Diffusion coeffic. (m^2/s)
CO_2 (*) (gas)	44.01	p*0.04401/(8.31451*T)	1x10^{-8}
$CaAl_2Si_2O_8$ (solid)	278.20	2740	1x10^{-9}
H2O (liquid)	18.02	1000	solvent
$CaCO_3$ (solid)	100.09	2710	1x10^{-9}
$AlSi_2O_5(OH)_4$ (solid)	258.16	2600	1x10^{-9}

(*) CO_2 is assumed to be an ideal gas at pressure *p* (Pa) and temperature *T* (K).

- Conservation equation is written in term of concentration per water volume of the porous media (Comsol Multiphysics® - Partially Saturated Porous Media definition).
- The porosity ⍰*p* is 0.25, water saturation grade *s* is 0.27 (relative humidity in the accelerated carbonation chamber is 65%).
- Therefore liquid volume fraction is *s* ϴ = 0.0675.
- CO_2 diffusion coefficient is assumed as 1x10^{-8} m^2/s and the CO_2 concentration in the accelerated carbonation chamber as 25% in volume.
- Reaction rate and the rate constants of chemical reactions are set with the standard values of Comsol Multiphysics® database.
- Temperature is 25 ^{o}C and the pressure is 1 atm.

Boundary conditions

- Set CO_2 concentration in vertical wall of sample ($r = R$) as 10.22 mol/m^3, obtained from %CO_2 concentration in the carbonation chamber.
- For the same wall, boundary conditions for the other dilutes species is mass flux equal to zero.
- Base surfaces are set as no mass flux for all chemical species.
- Axial symmetry is used on *z* axis of the concrete sample.
- Initial conditions for the species concentrations in the liquid fraction are 280 mol/m^3 for $CaAl_2Si_2O_8$ and zero for other reacting species.

Figure 3. Concentration profiles of reacting species after 28 days of carbonation (25% CO 2 , 65% RH, 25°C).

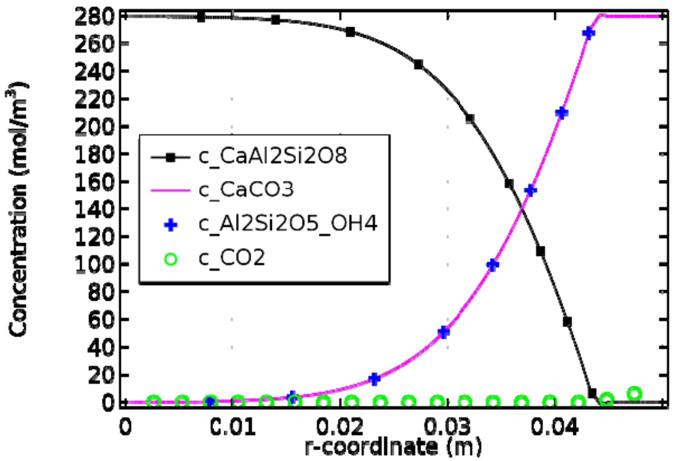
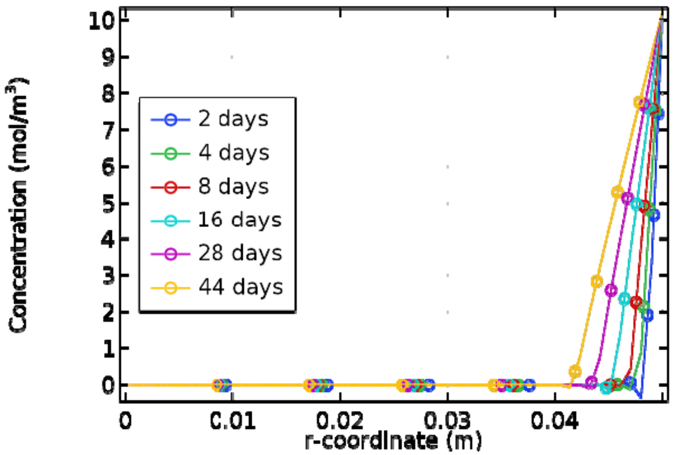


Figure 4. Concentration profiles of CO_2 in the concrete, for the carbonation times of Table 4 (25% CO_2, 65% RH, 25°C).



Results

Figure 5. Concentration profiles of $CaCO_3$ for the carbonation times of Table 4 (25% CO_2, 65% RH, 25°C).

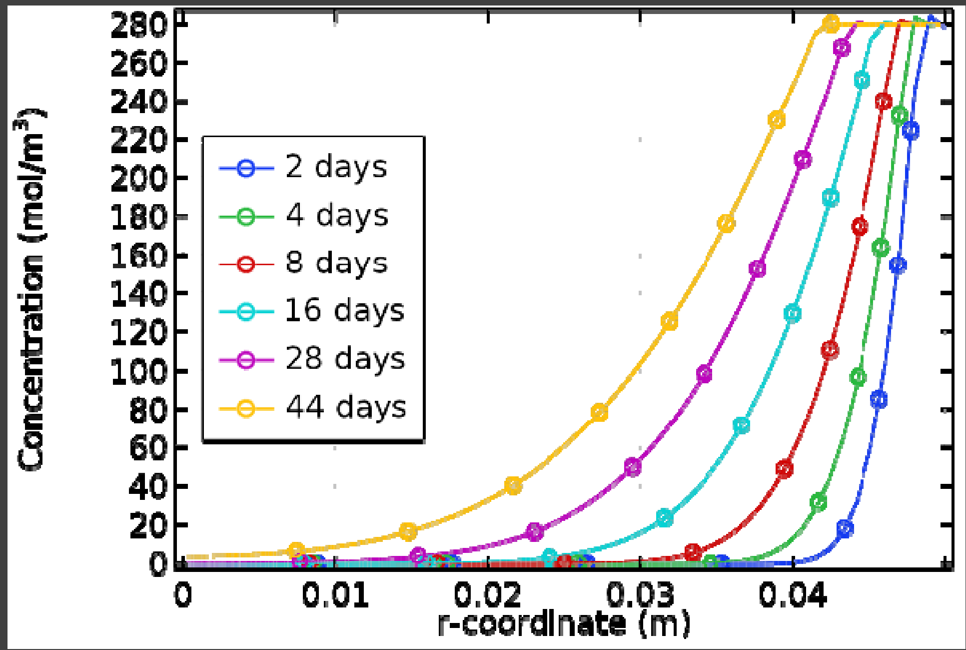


Figure 6. Carbonation depth in a sample of concrete, after 28 days of accelerated carbonation.

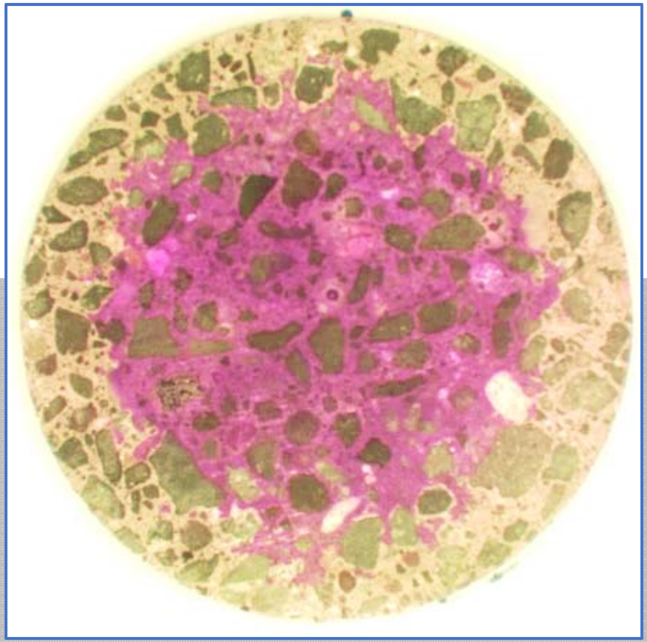


Table 4. Carbonation depth in the concrete.

Carbonation (days)	Experimental values of carbonation depth (mm)	Computational values of carbonation depth (mm)
2	4	3.5
4	6	4.5
8	8	6.5
16	10	9.5
28	12	12.5
44	15	17.0

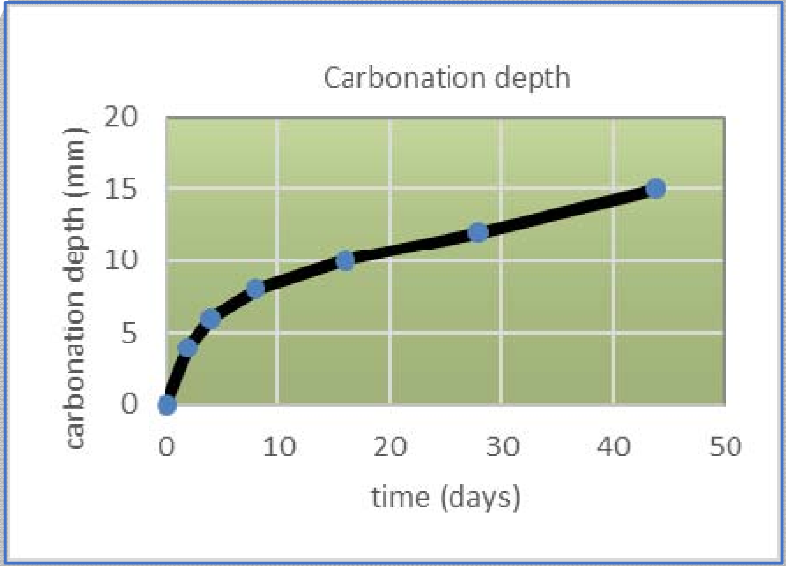


Figure 7. Carbonation depth with time in the concrete sample.

Conclusions

- A time dependent carbonation process of a concrete manufactured with pozzolanic cement has been modeled by using the Chemical Reaction Engineering Module of Comsol Multiphysics®.
- The numerical results give the carbonation front in time and species concentration in the carbonated concrete.
- Validation of results is made by comparing them with experimental testing in an accelerated carbonation chamber, under controlled conditions of relative humidity, CO_2 concentration and temperature.
- Computational results obtained with Comsol Multiphysics® are encouraging for a next study which will also include steel bar corrosion.

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Acknowledgements

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